Conventions, Accuracy Metrics, Classification, Regression

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IIT Gandhinagar

August 8, 2025

Outline

Demo

Comet browser and automation of tasks

Revision: What is Machine Learning

"Field of study that gives computers the ability to learn without being explicitly programmed" - Arthur Samuel [1959]

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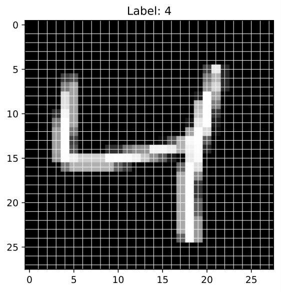
Let us work on the digit recognition problem.

Notebook: rule-based-vs-ml.html



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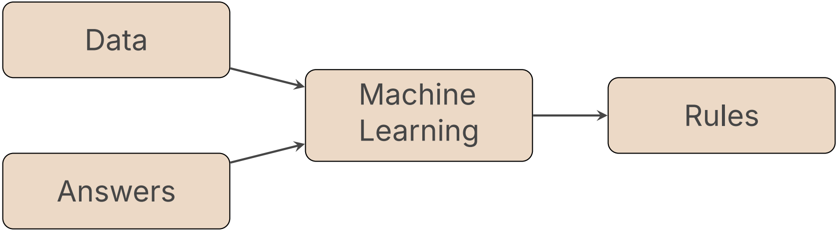
Traditional Programming vs Machine Learning

Traditional Programming

Machine Learning



Revision: What is Machine Learning

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T, as measured by P, improves with experience E." - Tom Mitchell

First ML Task: Grocery Store Tomato Quality Prediction

Problem statement: You want to predict the quality of a tomato given its visual features.

Dataset

Imagine you have some past data on quality of tomatoes.
What visual features do you think will be useful?

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Dataset

Imagine you have some past data on quality of tomatoes.
What visual features do you think will be useful?

- Size
- Colour

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Dataset

Imagine you have some past data on quality of tomatoes.
What visual features do you think will be useful?

- Size
- Colour
- Texture

Sample Dataset

Here is our example dataset with tomato features:

Sample	**Colour**	**Size**	**Texture**	**Condition**
1	Orange	Small	Smooth	Good
2	Red	Small	Rough	Good
3	Orange	Medium	Smooth	Bad
4	Yellow	Large	Smooth	Bad

Pop Quiz #1

Quick Quiz 1

Is the sample number a useful feature for predicting quality of a tomato?

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Quick Quiz 1

Is the sample number a useful feature for predicting quality of a tomato?
Answer: Usually no! Sample numbers are typically arbitrary identifiers and not meaningful features. Let us remove it.

Pop Quiz #1

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When could sample number be useful?

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Quick Quiz 1

When could sample number be useful?
In some cases, the sample number might be useful for tracking or auditing purposes. E.g. if some trucks are delayed during delivery, the sample number could help identify which batch of tomatoes was affected.

Useful Features

Useful Features

Let us modify our data table for now.

Colour	**Size**	**Texture**	**Condition**
Orange	Small	Smooth	Good
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Training Set

Colour	Size	Texture	Condition
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The training set consists of two parts:

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The training set consists of two parts:

1. Features (Input Variables)
2. Output or Response Variable

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Computers work with numbers! We need to encode categorical data numerically (one-hot encoding):

C0	C1	S0	S1	T0	T1	Good?
0	0	1	0	1	0	1
0	1	1	0	0	1	1
0	0	0	1	1	0	0
1	0	0	0	1	0	0

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Orange=00, Red=01, Yellow=10; Small=10, Medium=01, Large=00; Smooth=10, Rough=01; Good=1, Bad=0

More details on encoding later!

Data Matrix

C0	C1	S0	S1	T0	T1	Good?
0	0	1	0	1	0	1
0	1	1	0	0	1	1
0	0	0	1	1	0	0
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Data Matrix

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We call this data matrix $\mathbf{X}$, and the complete dataset $\mathcal{D}$:

1. Feature matrix ($\mathbf{X} \in \mathbb{R}^{n \times d}$) containing data of n samples each of which is d dimensional.

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For this example: $n = 4$ (samples), $d = 6$ (features after one-hot encoding)

Mathematical Notation Convention

Important: Mathematical Notation Convention

Matrices use **bold uppercase** ($\mathbf{X}$), vectors use **bold lowercase** ($\mathbf{y}$), scalars use regular letters (*n*, *d*)

Example: Examples from Our Tomato Dataset

- **Scalars**: $n = 4$ (samples), $d = 6$ (features), $y_1 = 1$

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For this example: $n = 4$, $d = 6$, so $\mathbf{X} \in \mathbb{R}^{4\times 6}$ and $\mathbf{y} \in \mathbb{R}^4$

Prediction Task

Estimate condition for unseen tomatoes (#5, 6) based on data set.

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Testing Set

Testing set is similar to training set, but, does not contain labels for output variable.

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Training set used to learn f, **Test set** for predictions

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Important: Key Question

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Key Points

Generalisation = Performance on **unseen data** from

Sample vs Population: A Simple Example

Example: Tomato Farm: 10,000 tomatoes ready for harvest

- **Population**: All 10,000 tomatoes

Key Challenge: Will your 100 tomatoes represent all 10,000? What if you only picked from one corner?
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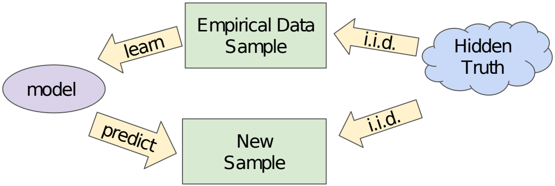

Image courtesy Google ML crash course

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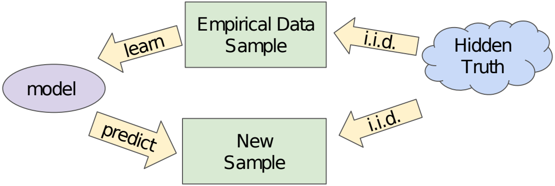

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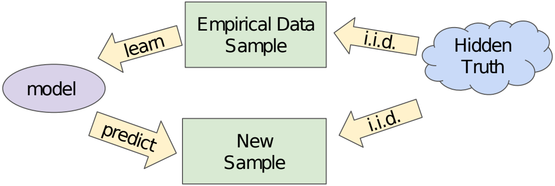

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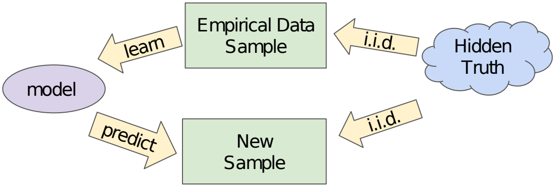

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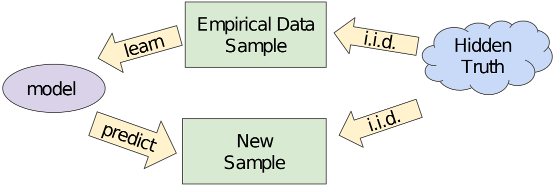

Image courtesy Google ML crash course

The ML Connection:

- **Population**: All possible tomato data (past, present, future)
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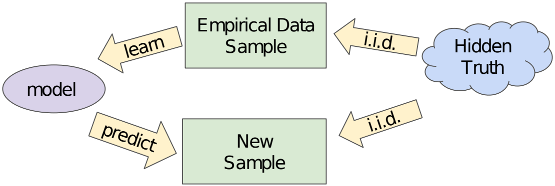

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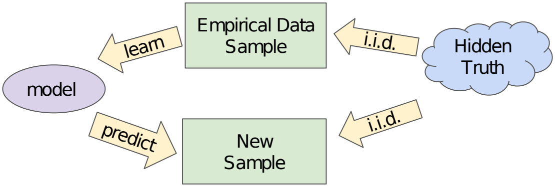

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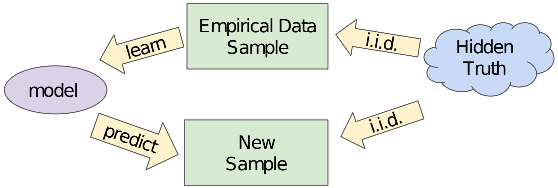

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- **Population**: All possible tomato data (past, present, future)
- **Training set**: Our 4 tomato samples (like picking from one area)
- **Test set**: 2 new samples (like picking from another area)

Generalisation goal: Will our model work on *all future tomatoes*, not just our small samples?

Second ML Task: Campus Energy Prediction

Regression Problem: Predicting continuous energy consumption (kWh)
Key factors: # People, Temperature

# People	Temp (°C)	Energy (kWh)
4000	30	30
4200	30	32
4200	35	40
3000	20	?
1000	45	?

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Difference from tomatoes: Energy is *continuous*, not categories

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    - How much rainfall will fall?

Pop Quiz #2

Quick Quiz 2

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- b) Classifying images as cat, dog, or bird
- c) Predicting house prices
- d) Determining if a tumor is malignant or benign

Pop Quiz #2 - Answer

Answer: c) House prices are continuous values - that's regression!

Now We Have Models - But How Good Are They?

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If our model predicts 5 tomatoes correctly and 3 incorrectly, is that good or bad? We need metrics!

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Coming up: Different metrics for classification vs regression problems

Back to Our Tomato Example: How Did We Do?

Let's say we trained our model and tested it on 5 new tomatoes:

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1	Good	Good
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Questions:

- How many did we get right? How many wrong?
- Is 3 out of 5 correct "good enough"?
- What if getting a bad tomato wrong is worse than getting a good tomato wrong?

Organizing Our Results

Let's organize the predictions in a simpler way:

$$\begin{array}{cc} \text{Model Predicted } (\hat{\mathbf{y}}) & \text{Actually Was } (\mathbf{y}) \\ \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Good} \\ \text{Bad} \end{pmatrix} & \begin{pmatrix} \text{Good} \\ \text{Good} \\ \text{Bad} \\ \text{Bad} \\ \text{Bad} \end{pmatrix} \end{array}$$

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Each row = one tomato's result
Goal: Create systematic ways to measure performance from these comparisons

Converting to Numbers for Computation

Remember: Computers work with numbers! Let's encode our categories:

Example: Binary Encoding

Bad = 0, **Good** = 1

Now our results become:

Predicted ($\hat{y}$) Ground Truth ($\mathbf{y}$)

$$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Ground Truth = The correct answers (what actually happened)

Accuracy: Measuring Overall Performance

How many predictions did we get exactly right?

Predicted $(\hat{\mathbf{y}})$ Ground Truth $(\mathbf{y})$

$$\begin{array}{c} \checkmark \\ \checkmark \\ \\ \\ \checkmark \end{array} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

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$$\text{Accuracy} = \frac{\text{Number of Correct Predictions}}{\text{Total Predictions}}$$

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For our example: Accuracy $= \frac{3}{5} = 0.6$ or 60%

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$$\text{Accuracy} = \frac{\sum_{i=1}^{n} \mathbf{1}[y_i = \hat{y}_i]}{n}$$

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- Both notations are mathematically equivalent and commonly used in ML literature

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Confusion Matrix

		Bad	Good
Pred	**Bad**	1	0
	Good	2	2

Confusion Matrix: Understanding the Four Outcomes

Confusion Matrix		Ground Truth	
		Positive	Negative
Predicted	Positive	TP	FP
	Negative	FN	TN

Definition: Four Outcomes

- **TP (True Positive):** Correctly predicted positive

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Confusion Matrix: Precision Focus

Confusion Matrix		Ground Truth		Row Totals
		Positive	**Negative**	
Predicted	**Positive**	TP	FP	**TP + FP**
	Negative	FN	TN	**FN + TN**
		TP + FN	**FP + TN**	**Total**

Example: Focus: Predicted Positives

$$\text{Precision} = \frac{\textbf{TP}}{\textbf{TP} + \textbf{FP}}$$

"Of all predicted positives, how many were actually positive?"

Confusion Matrix: Recall Focus

Confusion Matrix		Ground Truth		Row Totals
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		TP + FN	**FP + TN**	**Total**

Example: Focus: Actual Positives

$$\text{Recall} = \frac{\textbf{TP}}{\textbf{TP} + \textbf{FN}}$$

"Of all actual positives, how many did I catch?"

When Classes Are Imbalanced

Many datasets have unequal class distributions!

Example: Example: Medical Screening

Out of 1000 patients tested:

- **990** patients are healthy (negative class)

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Smart Classifier

Confusion Matrix		Ground Truth	
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	Neg	2	950

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- Precision: $\frac{8}{48} \approx 16.7\%$
- Recall: $\frac{8}{10} = 80\%$
- Accuracy: $\frac{8+950}{1000} = 95.8\%$

Precision vs Recall: The Trade-off

You often can’t have both high precision and high recall — improving one may reduce the other.

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Accuracy Metric: F1-Score

Confusion Matrix		Ground Truth	
		Positive	**Negative**
Predicted	**Positive**	TP	FP
	Negative	FN	TN

Example: F1-Score: Balancing Precision and Recall

$$\text{F1} = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

Accuracy Metric: Matthews Correlation Coefficient (MCC)

Confusion Matrix		Ground Truth	
		Positive	**Negative**
Predicted	**Positive**	TP	FP
	Negative	FN	TN

Example: MCC: Balanced Performance Measure

$$\text{MCC} = \frac{TP \cdot TN - FP \cdot FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

MCC Comparison: Dummy vs Smart Classifier

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Dummy Classifier

Confusion Matrix		Ground Truth	
		Pos	Neg
Pred	Pos	0	0
	Neg	10	990

MCC $= 0$ (denominator undefined; treat as 0)

MCC Comparison: Dummy vs Smart Classifier

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Confusion Matrix		Ground Truth	
		Pos	Neg
Pred	Pos	0	0
	Neg	10	990

$\text{MCC} = 0$ (denominator undefined; treat as 0)

Smart Classifier

Confusion Matrix		Ground Truth	
		Pos	Neg
Pred	Pos	8	40
	Neg	2	950

$$\text{MCC} = \frac{7600}{\sqrt{(48)(10)(990)(952)}} \approx \mathbf{0.26}$$

Confusion Matrix for multi-class classification

Notebook: confusion-mnist.html